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CONTROLLED EXCITATION OF THE OPTICAL MODE IN A COUPLED CHAIN

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Abstract
The comosite crystalline lattice is modelled as two coupled mutually-penetrating sublattices. With the help of the Internal Translation Symmetry principle the model was extended to the case of strongly nonlinear interacting sublattices. Dynamic models for the microscopic and macroscopic displacement fields include parameters, depending on the lattice deformation. This model is used for control of bifurcational lattice transformation, caused by external stress or deformation. Possibilities of controlled excitation of the optical mode of oscillation by means of the energy pumping from the side of the the acoustic mode based on feedback and non-feedback controls are analysed.

1 Introduction

In the papers (Aero *et al.*, 2005; Aero *et al.*, 2006) a highly nonlinear system of acoustic and optical oscillations in a composite crystalline lattice consisting of two sublattices is analyzed. The system is obtained as a generalization of the linear Carman–Born–Huang theory (Born and Huang, 1998). Large displacements of atoms up to structure stability loss and restructuring are admitted. It is shown that the system has nontrivial solutions describing movements of fronts, emergence of periodic structures and defects. Strong interaction of acoustic and optical modes of oscillation for media without center of symmetry is demonstrated and a possibility of energy-excitation of the optical mode by means of controlling torque applied to the ends of the lattice is examined. The feedback control law for optical mode excitation is derived based on Speed-Gradient method (Fradkov, 1979) and analyzed numerically. An easily realizable non-feedback version of control algorithm is proposed possessing similar properties. An important result of these works is demonstration of the possibility of purposeful excitation of the optical mode by means of torque applied to the ends of the lattice in a broad range of initial conditions. This means that application of control allows to eliminate or to reduce influence of initial conditions. Another conclusion is based on the well-known fact that static strains (deformations) influence phase state of smart materials. It implies that application of control for energy exchange between macroscopic deformation and microscopic degrees of freedom allows changing dynamics of phase transitions. In the present paper the similar results are obtained for the other important type of crystalline lattices.

The composite crystalline lattice under consideration is modeled as a two coupled mutually-penetrating sublattices. With the help of the "*Internal Translation Symmetry*" principle, introduced in (Aero, 2003; Aero, 2005), this model was extended to the case of strongly nonlinear interacting sublattices. Dynamic models for the microscopic and macroscopic displacement fields include parameters, depending on the lattice deformation. These parameters define nontrivial effects of interatomic barriers reduction, which influence on the structure and properties of the crystal is highly substantial. This model is used for control of bifurcational lattice transformation, caused by external stress or deformation. The example of the controlled excitation of microscopic mode (*the optical mode*) of oscillation by means of the energy pumping from the side of the macroscopic mode (*the acoustic mode*) is given.

For simplicity, the case when two sublattices may be united (merged in one) by shifting on some constant *structural vector* $\vec{u}_o$ (the lattice parameter) is considered in the sequel.

Two equations are known in the linear theory of crystalline lattice (Born and Huang, 1998): the "*acoustic mode*" $\vec{U}$ and the "*optical mode*" $\vec{u}$ equations, respectively. Introducing to the crystalline evolution theory the local topology by means of internal degrees of freedom (the field $\vec{u}$) seems to be efficient if the described below nonlinear extension of the linear approach is made.

Arbitrarily large sublattice displacements $\vec{u}$ may be introduced to the nonlinear theory of crystalline lattices if the theory is based on the additional component: the *translational symmetry*, which is typical for composite lattices but, nevertheless, it has not be considered so far in the solid-state physics framework. Evidently that the relative displacement of sublattices on the amount of one period (or on the integer number of periods) reproduces the initial pattern of the composite lattice. This means that the energy of the composite lattice should be a periodical function of the *stiff* displacement of sublattices $\vec{u}$, which is invariant with respect to this kind of translations.

2 General equations. One-dimensional, single-component case for centrosymmetrical crystals

2.1 Lattice dynamics

Introduce a displacement U of the center of inertia couple of atoms (of the *unit cell*) and the relative displacement u of the unit-cell atoms (this displacement is caused by changing of $\vec{u}_o$) as follows:

$$\vec{U}=\frac{m_1\vec{U}_1+m_2\vec{U}_2}{m_1+m_2},\quad \vec{u}=(\vec{U}_1-\vec{U}_2)/a, \tag{1}$$

where $\vec{U}_1$, $\vec{U}_2$ are displacements of the atoms of the first and the second sublattices, respectively, m_1 m_2 are corresponding atom masses, a denotes the *period* of the sublattices. To describe the fields $U(x,t)$, $u(x,t)$ in the one-dimensional case, write down the variational equations of motion.

Start from Lagrangian

$$L=\frac{1}{V}\int_0^t\int_V \big(\frac{1}{2}\rho\dot{U}_n\dot{U}_n+\frac{1}{2}\mu\dot{u}_n\,\dot{u}_n-D\big)\,\mathrm{d}t\,\mathrm{d}V, \tag{2}$$

where D denotes the energy of deformations and of structural changes. In the considered one-dimensional case an appropriate invariant expression for the energies of macro- and micro-deformations, taking into account their mutual interactions (the *nonlinear striction*) has a form:

$$D=\frac{\lambda}{2}(U_{,x})^2+\frac{k}{2}(u_{,x})^2+(p-S\,U_{,x})(1-\cos u) \tag{3}$$

(derivatives on time t are denoted by dots above variables, the spatial derivatives are indicated by commas in tensor indices). U and u stand for the components of the corresponding vector, not for its magnitude. The spatial derivatives $U_{,x}$ and $u_{,x}$ are macro- and microscopic gradients of U and v; λ, k are macro- and microscopic modules; S is a coefficient of the nonlinear striction, which is responsible for interaction between macro- and microscopic fields); $2p$ is an interatomic potential barrier of an undistorted lattice (i.e. an activation energy of the unit-cell atomic bond).

For practice, the most important case of one-dimensional lattice is a *flat layerwise microstructure*. A particular kind of this structure is the nanolaminate, appearing in several nanotechnologies during sintering and tempering of thin hardened foil under crystallization.

The corresponding variational equations of motion are as follows:

$$\rho_1\ddot{U}=\lambda U_{,xx}-S(1-\cos u)_{,x}, \tag{4}$$
$$\rho_2\ddot{u}=ku_{,xx}-(p-SU_{,x})\sin u. \tag{5}$$

2.2 Bifurcation point and opportunities for optical mode excitation

In is worth to mention that, as it is seen from (5), there exists a *bifurcation point* for u. At this point the factor outside $\sin u$ becomes zero as

$$p-SU_{,x}=0. \tag{6}$$

This coefficient (the left-hand side of (6)) may be referred as an *efficient interatomic potential barrier*, depending on the deformation $U_{,x}$. Condition (6) defines the point of a cardinal structure transformation of a crystal, caused by overcoming the potential barrier, holding the crystal structure.

It follows from (4) that for $u=\pi$ there exists the next one threshold – the *tension threshold*. It corresponds to the following equalities:

$$\sigma=\sigma_t,\quad \sigma_t=\lambda U_x-2S. \tag{7}$$

These two thresholds separate three areas of a crystal structural state. Control of crystal properties may be achieved by overcoming the reconfiguration barriers by means of external tensions or deformations. Condition (6) defines the first reconfiguration threshold. For positive material parameters p and S, this threshold is related to positive deformations $U_{,x}$, i.e. is related to *tension*. Because deformations should satisfy the other equation, the bifurcation control may be reached by changing macro-displacements or forces at the crystal bounds. The second threshold, defined by condition (7), is achieved by means of lower level of tension.

Due to coupling between acoustic and optical modes in (4), (5), and the microscopic boundary conditions may be equal to zero: the microscopic field will certainly arise inside the crystal body. In the lattice dynamics this effect is disclosed as an *excitation* of the microscopic (*optical*) mode by means of the *acoustic* mode merely.

Conditions (6), (7) show that there exists an *excitation threshold* on microforce tensile strain for zero boundary conditions. If these conditions are nonzero, the threshold is displaced or even may disappear. At the last case the microdisplacements are excited by means of the perturbation of boundary conditions exclusively.

3 Examination of lattice dynamics

In this Section the results of numerical examination the lattice dynamics are presented. The lattice model and its parameters, used for examinations are given in Sec. 3.1. Lattice behavior under constant microforce is studied in 3.2. Section 3.3 is devoted excitation the optical mode by means of the feedback control.

3.1 Model for the numerical examinations

For taking into consideration the *energy dissipation*, inherent to crystalline lattices, introduce the *dissipative* terms $\dot{U}$ and $\dot{u}$ in the model (4), (5) and rewrite this model as follows:

$$\begin{cases} \tilde{s}\ddot{U} + \tilde{\mu}\dot{U} = U_{,xx} + \tilde{\beta}\sin(u)u_{,x} \\ s\ddot{u} + \mu\dot{u} = ku_{xx} - p(1 - \beta U_{,x})\sin u, \end{cases} \tag{8}$$

where $\tilde{s}$, $\tilde{\beta}$, $\tilde{\mu}$, s, μ, k are lattice model parameters.

In our study, the following parameter values were taken: $\tilde{s} = 0.9$, $\tilde{\beta} = 2$, $\tilde{\mu} = 1$, $s = 2.5$, $\mu = 1$, $k = 0.1$, $p = 1 > 1$. The initial conditions for first time derivatives of both acoustic and optical modes were zero. The PDE (8) were solved numerically via the finite difference method. For transforming the PDE to ordinary differential equations (ODE) the following approximation was used:

$$\frac{\partial u}{\partial \xi} = \frac{1}{\Delta}(u_{i+1} - u_i), \quad \frac{\partial U}{\partial \xi} = \frac{1}{\Delta}(U_{i+1} - U_i),$$
$$\frac{\partial^2 u}{\partial \xi^2} = \frac{1}{\Delta^2}(u_{i+1} - 2u_i + u_{i-1}),$$
$$\frac{\partial^2 U}{\partial \xi^2} = \frac{1}{\Delta^2}(U_{i+1} - 2U_i + U_{i-1}).$$

where an argument $\xi \in [0, 1]$ denotes the scaled spatial coordinate x. For $i = 1$ the left boundary conditions were taken instead of u_{i-1}, U_{i-1}, and the right boundary conditions were taken instead of u_{i+1}, U_{i+1} for $i = n$. The grid distance Δ for the PDE solving was taken as $\Delta = 1/n$, where $n = 50$.

3.2 Lattice behavior under constant microforce

Several simulations were made to examine the lattice behavior for the case when microforce and microdisplacement are constant on time. To this end, the boundary conditions for acoustic mode F_1, F_2 and optical mode f_1, f_2 were taken constant on t and, opposite in sign: $F_2 = -F_1$, $f_2 = -f_1$. The different values of F_1, f_1 were taken in the simulation runs.

Sections of the optical mode $u(\cdot, t)$ for different instants t are plotted in Figs. 1, 3, 6. The plots depicted in Fig. 1 correspond to the case $F_1 = -5$, $f_1 = f_2 = 0$, $U(\cdot, 0) = 0$, $u(\cdot, 0) = \pi/50$. It is seen that the optical mode tends to zero. If the magnitude of F_1 exceeds some *bifurcation point* (this point is defined by condition (7)), the optical mode is excited. This case is demonstrated in Fig. 3 for $F_1 = -15$. The spatio-temporal plots are shown in Fig. 2, 4, respectively. The "generalized" phase plot in the space of integrated intensity of the optical mode $\int_0^1 u(\xi, t)\,\mathrm{d}\xi$ and its time derivative $\left(\int_0^1 u(\xi, t)\,\mathrm{d}\xi, \int_0^1 \dot{u}(\xi, t)\,\mathrm{d}\xi \right.$ for $F_1 = -15$, is depicted in Fig. 5. Case when the tension force exceeds the threshold ($F_1 = -15$) and non-zero torque is applied ($f_1 = f_2 = 1$) is demonstrated in Fig. 6. It is seen that the torque f_1 leads to dissymmetry of the optical mode.

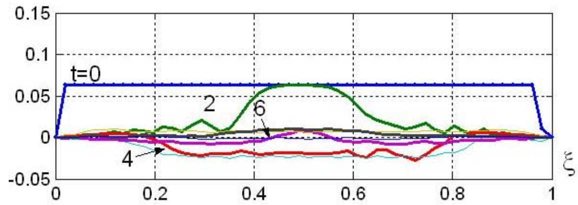

Figure 1. $F_1 = -5, f_1 = f_2 = 0, U(\cdot, 0) = 0, u(\cdot, 0) = \pi/50$. Optical mode vanishes.

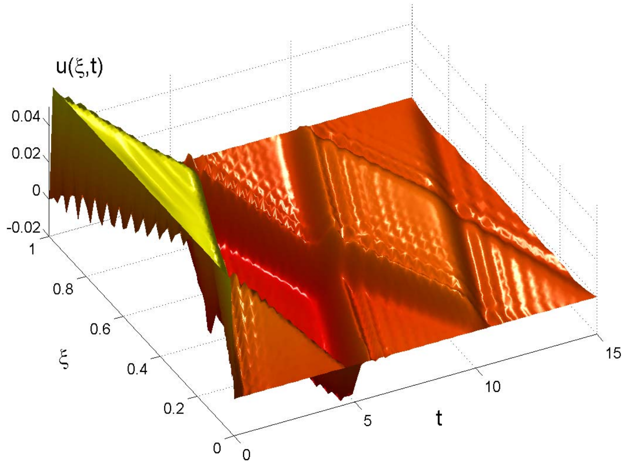

Figure 2. Spatio-temporal plot $u(\xi, t)$. $F_1 = -5, f_1 = f_2 = 0, U(\cdot, 0) = 0, u(\cdot, 0) = \pi/50$. Optical mode vanishes.

Dependence of the optical mode intensity on the tension force F_1 is demonstrated in Fig. 7. The following indices $Q_{u,\text{peak}} = \sup_t \left(\sup_\xi (|u(\xi, t)|) \right)$, $Q_{\Sigma u,\text{peak}} = \sup_t \left(\int_0^1 u(\xi, t)\,\mathrm{d}\xi \right)$, $Q_{u,\infty} = \sup_\xi \left(\lim_{t\to\infty} |u(\xi, t)| \right)$, and $Q_{\Sigma u,\infty} = \int_0^1 \left(\lim_{t\to\infty} u(\xi, t) \right)\mathrm{d}\xi$ are plotted as functions of F_1. The plots show that if $F_1 < 0$ and its magnitude exceeds the bifurcation value $F_1^* \approx -11$, the optical mode is excited. This result complies with the theoretical statements, see (7) and the related comments.

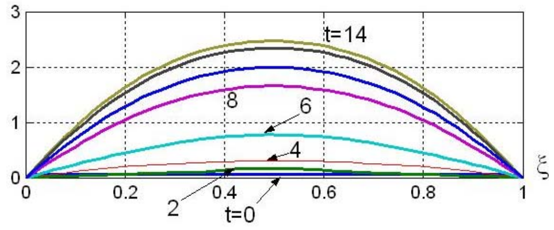

Figure 3. $F_1 = -15$, $f_1 = f_2 = 0$, $U(\cdot,0) = 0$, $u(\cdot,0) = \pi/50$. Optical mode is excited.

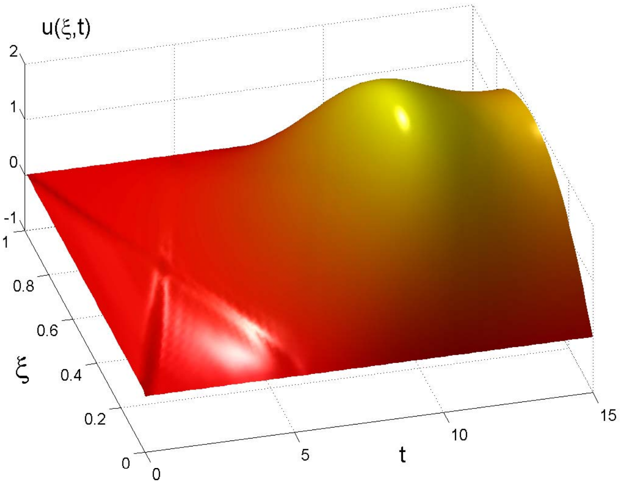

Figure 4. Spatio-temporal plot $u(\xi,t)$. $F_1 = -15$, $f_1 = f_2 = 0$, $U(\cdot,0) = 0$, $u(\cdot,0) = \pi/50$. Optical mode is excited.

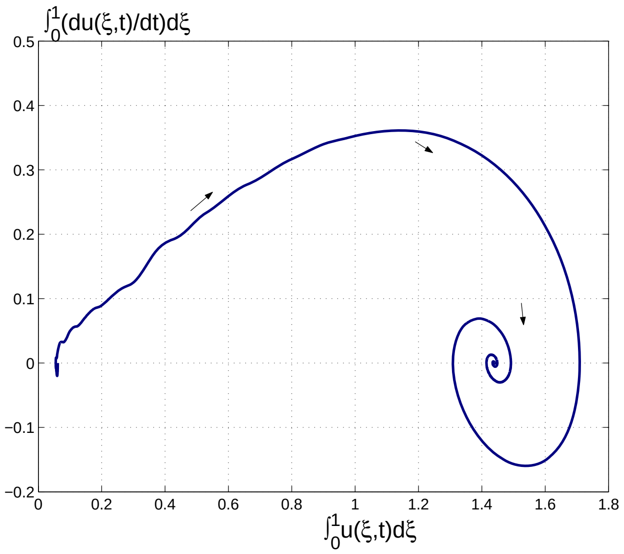

Figure 5. "Generalized" phase plot. $F_1 = -15$, $f_1 = f_2 = 0$, $U(\cdot,0) = 0$, $u(\cdot,0) = \pi/50$. Optical mode is excited.

3.3 Optical mode excitation by feedback control

Consider the possibilities of excitation the optical mode applying the feedback controlled tension microforce. To this end let us apply the Speed-gradient (SG) design method (Fradkov, 1979; Fradkov and Pogromsky, 1998; Fradkov, 2005; Fradkov, 2007) taking the

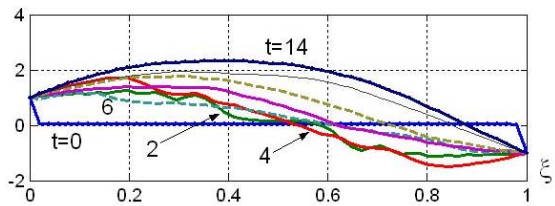

Figure 6. $F_1 = -15$, $f_1 = f_2 = 1$. $U(\cdot,0) = 0$, $u(\cdot,0) = \pi/50$. Optical mode is excited; dissymmetry of the optical mode is observed.

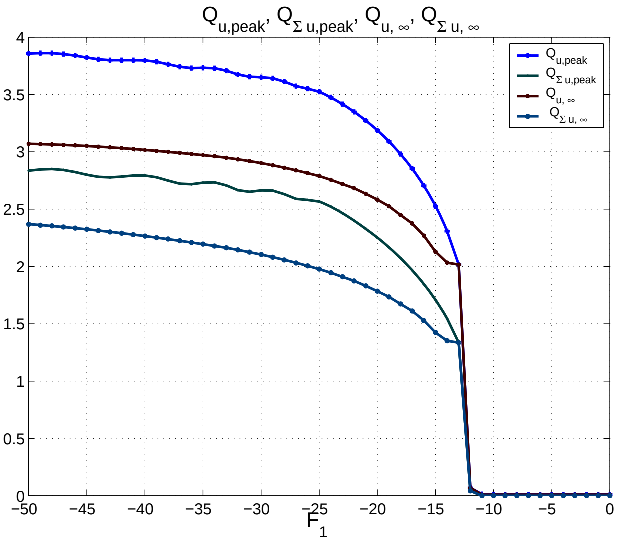

Figure 7. Optical mode intensity v.s. level of the tension force F_1. Bifurcation value $F_1 = -11$.

goal function $Q(u)$ in the form

$$Q(u) = \left(\int_0^1 u(\xi,t)\, \mathrm{d}\xi \right)^2. \quad (9)$$

The function (9) may be considered as some "integral" characteristic of the optical mode.

Applying the SG algorithm in the *relay form* and making some simplifying assumptions we obtain the following excitation feedback control law:

$$F(u,\dot{u}) = F_m \operatorname{sign}\left(\int_0^1 u(\xi,t)\, \mathrm{d}\xi \cdot \int_0^1 \dot{u}(\xi,t)\, \mathrm{d}\xi \right), \quad (10)$$

where F_m is the magnitude of the tension microforce.

Numerical evaluation results for $F_m = 15$ are plotted in Figs. 8, 9. It is seen from the plots, the feedback control law (10) excites the oscillating optical mode. The tension force $F_1(t)$ in the steady-state mode has a shape of a "square waveform". The time histories of

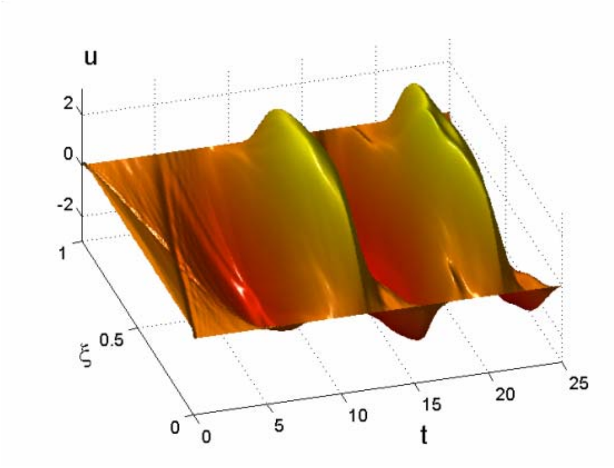

Figure 8. Spatio-temporal plot $u(\xi, t)$. Optical mode excitation by means of the feedback control (10), $F_m = 15$.

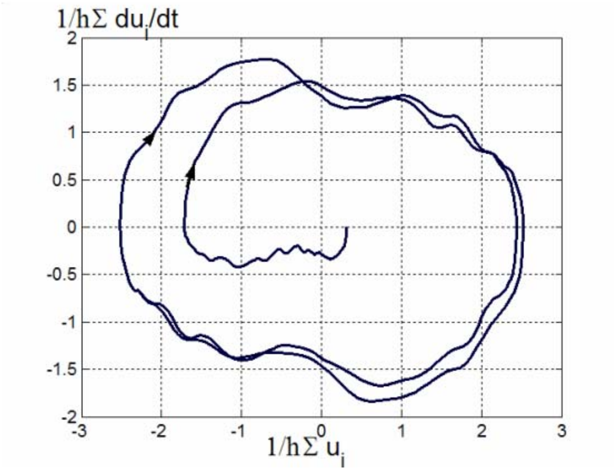

Figure 9. "Generalized" phase plot. Optical mode excitation by means of the feedback control (10), $F_m = 15$.

$F_1(t)$ and the stress $\sigma|_{\xi=0.5}(t)$, see (7), are plotted in Fig. 10. The numerical examinations show that the

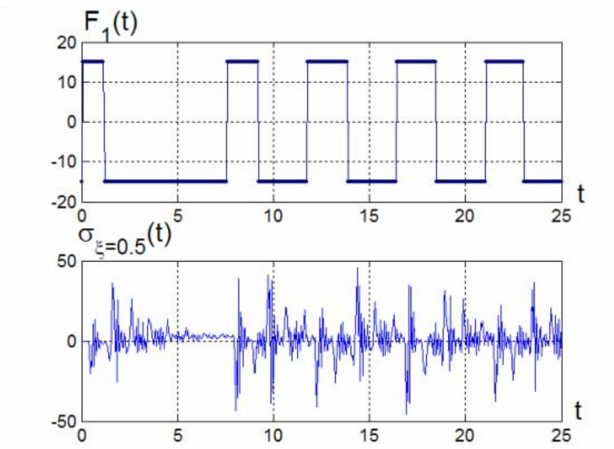

Figure 10. $F_1(t)$ and $\sigma(t)$ time histories; $F_m = 15$.

"threshold value" for feedback control magnitude F_m is approximately $F_m^* = 7$. The corresponding phase plot is depicted in Fig. 11. For the less values of F_m no excitation of the optical mode occurs. It should be noticed that the threshold F_m^* for feedback control is about 0.64 of the threshold F_m^* for constant microforce, see Sec. 3.2.

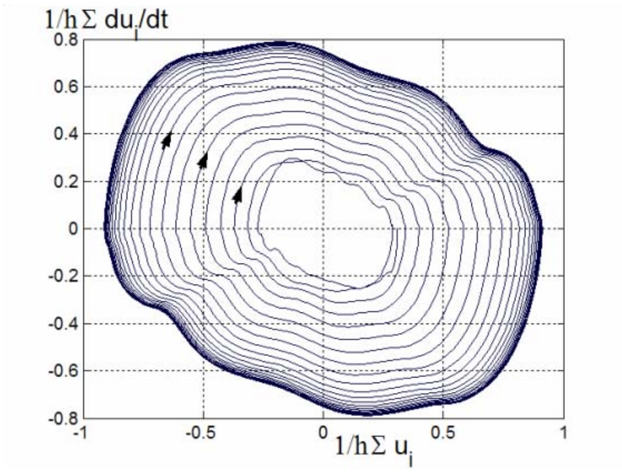

Figure 11. "Generalized" phase plot. Optical mode excitation by means of the feedback control (10), $F_m = 7$.

4 Conclusions

Excitation of the optical mode by means of acoustic one may be assured if the tension force F_1 is negative and large enough in magnitude. The constant torque f_1 leads to dissymmetry of the optical mode. The SG feedback control in the relay form leads to oscillations of the optical mode. The threshold for feedback control is about two times less those for constant microforce.

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